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DFT Calculations for Planning the Synthesis of More Efficient Devices Performing Artificial Photosynthesis

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DFT calculations for planning the synthesis of more efficient devices performing artificial photosynthesis

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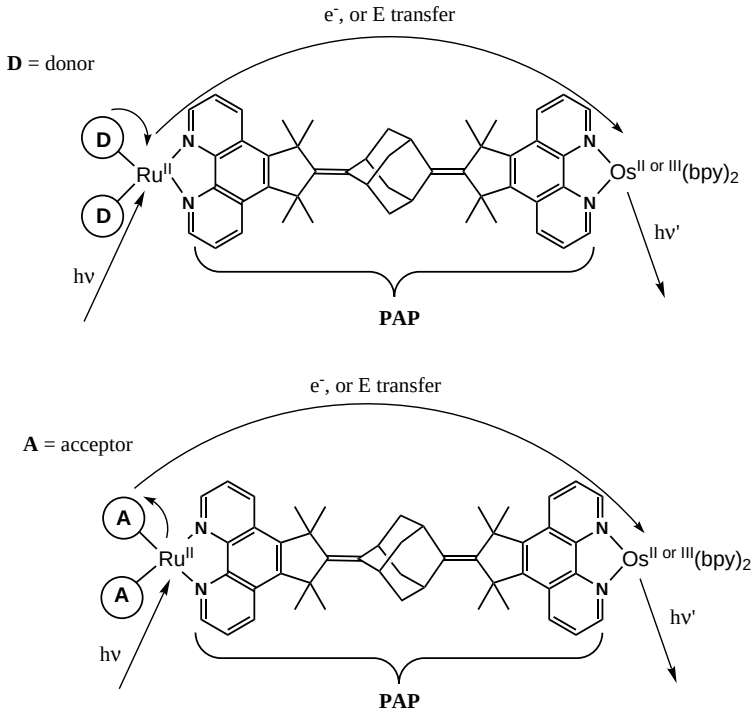
Energy and electron transfer processes are very important since they are at the base of many biological phenomena, such as photosynthesis. The system showed below is an example of an inorganic device performing efficient photoinduced energy and electron transfer processes ($k_{\mathrm{en}} = 5.2 \times 10^7 s^{-1}, k_{\mathrm{el}} = 7.2 \times 10^6 s^{-1}$, [1]). The introduction of appropriate donor and acceptor units on the Ru(II) center can improve the lifetime of the charge/energy transfer state, resulting in a much longer and efficient storage of energy. Ab initio (DFT) calculations were made in order to predict the best donor and acceptor ligands for the synthesis of the target molecules.



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[1] V. Balzani, F. Barigelletti, P. Belser, S. Bernhard, L. De Cola, and L. Flamigni, J. Phys. Chem. **1996**, *100*, 16786.